Ethanone, 1-(3-hydroxyphenyl)-121-71-1 | DTXSID5059533

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 3.55 days

Global applicability domain: Outside

Local applicability domain index: 3.88e-01

Confidence level: 9.36e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5 Predicted: 3.17

Image not found

Propylbenzene Measured: 24.3 Predicted: 4.02

Image not found

3-Ethyltoluene Measured: 12.5 Predicted: 3.26

Image not found

1-Ethyl-2-methylbenzene

Measured: 24.3 Predicted: 3.88

Image not found

4-Ethyltoluene Measured: 24.3 Predicted: 3.95